On the Relation Between Information and Power in Stochastic Thermodynamic Engines

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Dec 15, 2021

Outline

- Background on stochastic thermodynamics
- 2nd law of thermodynamics and Wasserstein geometry
- Generalization when continuous-time measurements are available

What is stochastic thermodynamics?

- study thermodynamics at the level of individual particle and far from equilibrium
- a branch of non-equilibrium statistical physics (developed over the last few decades)

Applications:

- biological molecular machines (e.g. kinesin and myosin)
- artificial nano devices (energy of order $k_B T$)

Questions:

- minimum dissipation over finite time transitions
- maximum power from a stochastic thermodynamic engine
- how to extract power from noisy measurements (this work)

Tools from control can be used to formulate and study these questions

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Overdamped Langevin eq.

$$\gamma \mathrm{d}X_t = -\nabla_x U(t, X_t)\mathrm{d}t + \sqrt{2D}\mathrm{d}B_t$$

- a particle in a medium of temperature T
- manipulated by external potential $U(t,x)$
- γ is the viscosity coefficient
- $D = \gamma k_B T$ is the diffusion constant

Potential $U(t,x)$ is controlled to achieve certain objectives, e.g. extract work

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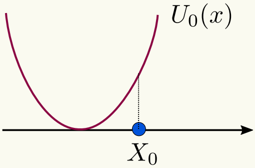

Energy:

$$E = U_0(X_0)$$

Work: energy exchange by changing the potential (with external agent)

$$W = U_1(X_0) - U_0(X_0)$$

Heat: energy exchange when particle moves (with medium)

$$Q = U_1(X_1) - U_1(X_0)$$

1st law: conservation of energy

$$\Delta E = Q + W$$

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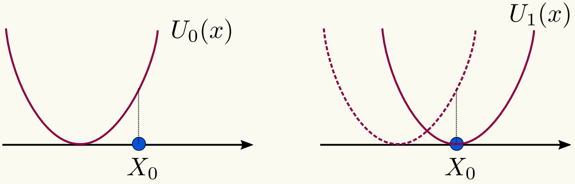
Stochastic thermodynamic

Definitions of work and heat for individual particle



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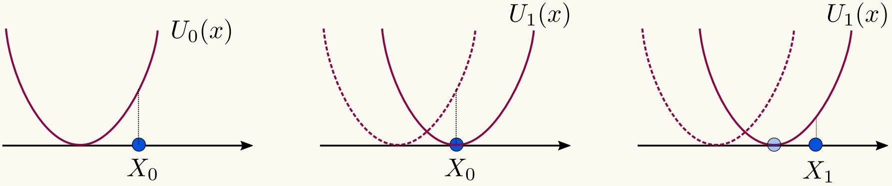

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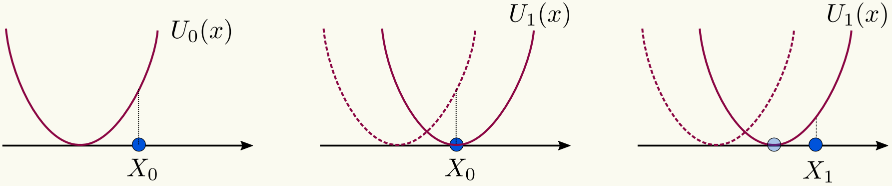

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Stochastic thermodynamic
Definitions of work and heat in continuous-time

Consider continuous-time trajectory $\{X_t; t \in [0, t_f]\}$ and $\{U(t, \cdot); t \in [0, t_f]\}$

- change in energy

$$\mathrm{d}E_t = \mathrm{d}U(t, X_t) = \frac{\partial U}{\partial t}(t, X_t)\mathrm{d}t + \nabla_x U(t, X_t) \circ \mathrm{d}X_t$$

- Work

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- heat

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$$\Delta E = W + Q$$

- Average energy

$$\mathcal{E}_t = \mathbb{E}[U(t, X_t)] = \int U(t, x) p(t, x) \mathrm{d}x$$

- Average work

$$\mathcal{W} = \int_0^{t_f} \mathbb{E}[\frac{\partial U}{\partial t}(t, X_t)] \mathrm{d}t = \int_0^{t_f} \int \frac{\partial U}{\partial t}(t, x) p(t, x) \mathrm{d}x \mathrm{d}t$$

- Average heat

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$p(t, x)$ is probability dist. of X_t given by Fokker-Planck eq.

$$\frac{\partial p}{\partial t} = \frac{1}{\gamma} \nabla \cdot (p \nabla U) + \frac{k_B T}{\gamma} \Delta p$$

- Average energy

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Entropy:

$$\mathcal{S}(p) = -\int \log(p(x))p(x)\mathrm{d}x$$

Free energy:

$$\mathcal{F}(p, U) = \int U(x)p(x)\mathrm{d}x - k_B T S(p)$$

Second law:

$$\Delta\mathcal{S}_{\text{tot}} = \Delta\mathcal{S}_{\text{sys}} + \Delta\mathcal{S}_{\text{env}} \geq 0 \quad \Longleftrightarrow \quad \mathcal{W} - \Delta\mathcal{F} = \mathcal{W}_{\text{diss}} \geq 0$$

Question: how to prove and refine 2nd law for overdamped Langevin eq.?

Background on Wasserstein geometry

- Consider the curve $\{p(t,x); t \in [0,1]\}$ in the space of probability distributions
- A unique vector-field $\nabla\phi(t,x)$ is associated with the curve such that

$$\frac{\partial p}{\partial t} + \nabla \cdot (p \nabla \phi) = 0$$

- The Wasserstein Riemannian metric at each point

$$\|\frac{\partial p}{\partial t}\|_{\mathrm{W}}^2 := \int \|\nabla\phi\|^2 p \mathrm{d}x$$

- The length of the curve is

$$\mathsf{length}_{\mathrm{W}}(p_{[0,1]}) := \int_0^1 \|\frac{\partial p}{\partial t}\|_{\mathrm{W}} \mathrm{d}t$$

- The length of the geodesic connecting p_0 and p_1 is the 2-Wasserstein distance

$$\mathrm{W}_2(p_0,p_1) := \min\{\mathsf{length}_{\mathrm{W}}(p_{[0,1]}); \text{with fixed end-points}\}$$

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- Free energy is also relative entropy with respect to equilibrium $p_{\text{eq}} = \frac{1}{Z} e^{-\frac{1}{k_B T} U}$

$$\mathcal{F}(p, U) = k_B T D(p \| p_{\text{eq}}) + k_B T \log(Z)$$

- If U is constant, the time-derivative of free energy along Fokker-Planck flow is

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}(p, U) = -\gamma \| \frac{\partial p}{\partial t} \|_{\mathrm{W}}^2$$

- When U is time-varying,

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}(p, U) = \int \frac{\partial U}{\partial t} p \,\mathrm{d}x - \gamma \| \frac{\partial p}{\partial t} \|_{\mathrm{W}}^2$$

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2nd law and Wasserstein geometry

2nd law with no measurements

For the over-damped Langevin eq., we have the identity

$$\mathcal{W} - \Delta\mathcal{F} = \gamma \int_0^{t_f} \|\frac{\partial p}{\partial t}\|_{\mathrm{W}}^2 \mathrm{d}t$$

and the bound

$$\mathcal{W} - \Delta\mathcal{F} \geq \frac{\gamma}{t_f}\mathsf{length}_{\mathrm{W}}(p_{[0,t_f]}) \geq \frac{\gamma}{t_f}\mathrm{W}_2^2(p_0, p_f)$$

- This is refinement of the second law for finite-time non-equilibrium transitions
- The bound is achieved when moving with constant velocity along the geodesic
- RHS converges to zero as transition time $t_f \to \infty$ (quasi-static limit)

E. Aurell, C. Mejía-Monasterio, and P. Muratore-Ginanneschi, Optimal protocols and optimal transport in stochastic thermodynamics, Phys. Rev. Lett, 2011
Y. Chen, T. Georgiou, and A. Tannenbaum, "Stochastic control and non-equilibrium thermodynamics: fundamental limits," IEEE TAC, 2019.
R. Fu, A. Taghvaei, Y. Chen, and T. T. Georgiou, "Maximal power output of a stochastic thermodynamic engine", Automatica, 2021.

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Model:

$$\gamma \mathrm{d}X_t = -\nabla U(t, X_t)\mathrm{d}t + \sqrt{2D}\mathrm{d}B_t$$
$$\mathrm{d}Z_t = h(X_t)\mathrm{d}t + \sigma_v \mathrm{d}V_t$$

- $h(x)$ is the observation function
- V_t is Brownian motion representing noise in measurements
- σ_v is the strength of the noise

Information structure:

- potential function $U^{\mathcal{Z}_t}(t, x)$ is allowed to depend on the history of observations
- $\mathcal{Z}_t$ is the filtration generated by $\{Z_s; s \in [0, t]\}$
- information may be used to violate 2nd law (Maxwell's demon)

Objective: refine the 2nd law when we have access to noisy measurements

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Expected work conditioned on measurements:

$$\begin{aligned}\mathbb{E}[W|\mathcal{Z}_{t_f}] &= \int_0^{t_f} \mathbb{E}[\frac{\partial U^{\mathcal{Z}_t}}{\partial t}(t, X_t)|\mathcal{Z}_t]\mathrm{d}t \\ &= \int_0^{t_f} \int \frac{\partial U^{\mathcal{Z}_t}}{\partial t}(t, x)q(t, x)\mathrm{d}x\mathrm{d}t\end{aligned}$$

- where $q(t, x)$ is the density for the conditional distribution $P_{X_t|\mathcal{Z}_t}$
- It evolves according to the Kushner-Stratonovich eq.

$$\mathrm{d}q = \nabla \cdot (q\nabla\phi)\mathrm{d}t + \frac{1}{\sigma_v^2} q(h - \hat{h})(\mathrm{d}Z_t - \hat{h}\mathrm{d}t)$$

- where $\phi = \dfrac{1}{\gamma}(U + k_B T \log(q))$ and $\hat{h} = \int hq\mathrm{d}x$.

Entropy production for conditional distribution:

$$\mathrm{d}\mathcal{F}(U^{\mathcal{Z}_t}, q) = \left[\int \frac{\partial U^{\mathcal{Z}_t}}{\partial t} q \,\mathrm{d}x - \gamma \int \|\nabla\phi\|^2 q \,\mathrm{d}x + \frac{k_B T}{2\sigma_v^2} \int (h - \hat{h}_t)^2 q \,\mathrm{d}x\right] \mathrm{d}t + \text{(Martingale)}$$

- First term is related to conditional expectation of work $\mathrm{d}\mathbb{E}[W|\mathcal{Z}_t]$
- Second term $\int \|\nabla\phi\|^2 q\mathrm{d}x \geq \|\frac{\partial p}{\partial t}\|_W^2$ where p is the density for P_X
- Third term is related to mutual information between particle trajectory and observation signal (Duncan, 1970)

$$\mathcal{I}(X_{[0,t_f]}, Z_{[0,t_f]}) = \frac{1}{2\sigma_v^2} \int_0^{t_f} \mathbb{E}[(h(X_t) - \hat{h}_t)^2]\mathrm{d}t$$

- Fourth term involves the innovation process and disappears after expectation

2nd law for continuous measurements

Main result

Consider the over-damped Langevin dynamics with access to continuous measurements. Assume the initial and terminal potential functions are fixed to U_0 and U_f respectively. Then,

$$\mathcal{W} - \Delta\mathcal{F} \geq \frac{\gamma}{t_f} \mathrm{W}_2^2(p_0, p_{t_f}) - k_B T(\mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]}) - \mathcal{I}(X_{t_f}, Z_{t_f}))$$

- Extra term is the mutual information between the particle location and observations as well as the remaining information that has not been used
- Information can be used to extract work over a cycle ($\Delta\mathcal{F} = 0$) (information engines)

$$-\mathcal{W} \leq k_B T \mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]})$$

- The efficiency of a information engine is defined as

$$\eta = \frac{\text{extracted work}}{\text{available information}} = \frac{-\mathcal{W}}{k_B T \mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]})}$$

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2nd law for continuous measurements

Main result

Consider the over-damped Langevin dynamics with access to continuous measurements. Assume the initial and terminal potential functions are fixed to U_0 and U_f respectively. Then,

$$\mathcal{W} - \Delta\mathcal{F} \geq \frac{\gamma}{t_f}\mathrm{W}_2^2(p_0, p_{t_f}) - k_B T(\mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]}) - \mathcal{I}(X_{t_f}, Z_{t_f}))$$

- Extra term is the mutual information between the particle location and observations as well as the remaining information that has not been used
- Information can be used to extract work over a cycle ($\Delta\mathcal{F} = 0$) (information engines)

$$-\mathcal{W} \leq k_B T \mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]})$$

- The efficiency of a information engine is defined as

$$\eta = \frac{\text{extracted work}}{\text{available information}} = \frac{-\mathcal{W}}{k_B T \mathcal{I}(X_{[0,t_f]}; Z_{[0,t_f]})}$$

Analysis in linear Gaussian setting

Assumptions:

- potential $U(t,x) = \frac{q_0}{2}(x - r_t)^2$ is quadratic
- r_t is the control variable
- observation function $h(x) = x$ is linear

Stochastic optimal control problem:

$$\mathcal{W}^* = \min_{r(\cdot)\in\mathcal{F}_{\mathcal{Z}}} \mathbb{E}\left[\int_0^{t_f} \frac{\partial U}{\partial t}(t, X_t)\mathrm{d}t\right]$$

Solution

- optimal control law $r_t = (\frac{1}{2} - P_t)\mathbb{E}[X_t|\mathcal{Z}_t]$ where P_t solves backward Ricatti eq.
- maximum work output

$$-\mathcal{W}^* = -\frac{q_0}{2\sigma_v^2}\int_0^{t_f} P_t \mathsf{Cov}(X_t|\mathcal{Z}_t)\mathrm{d}t$$

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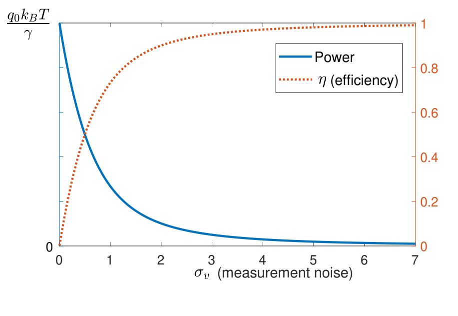
The steady state average power and efficiency are

$$\lim_{t_f\to\infty} \frac{-\mathcal{W}^*}{t_f} = \frac{q_0 k_B T}{\gamma}\frac{1}{\mathsf{SNR}}(\sqrt{1+\mathsf{SNR}}-1)^2$$
$$\lim_{t_f\to\infty} \eta = \frac{2}{\mathsf{SNR}}(\sqrt{1+\mathsf{SNR}}-1)$$

where $\mathsf{SNR} = \dfrac{2\gamma k_B T}{q_0^2\sigma_v^2}$



Concluding remarks

Summary:

- Tight bounds on maximum work from continuous stream of measurements
- Tools from optimal control, nonlinear filtering, and optimal transportation
- Optimal control law to extract maximum work in linear Gaussian setting

Open questions:

- Beyond linear Gaussian setting $\rightarrow$ POMDP
- Fluctuation theorems
- Other stochastic models (finite-state space case)

$\boxed{\text{Thank you for your attention!}}$